

Exhibit B

W0299

Automated Molecular Replacement. Charles R. Kissinger and Bradley A. Smith, Pfizer, Inc. 11099 North Torrey Pines Rd., La Jolla, CA 92037.

New molecular replacement (MR) techniques have made it feasible to screen large databases of protein structures or structural fragments to extract the best available search model for a particular MR problem. The use of stochastic search techniques, such as simulated annealing or evolutionary algorithms, to carry out rapid six-dimensional (or higher) MR searches has proven to be a robust method for solving MR problems. This approach can be extended to make large-scale, highly automated search-model screening practical. We have developed a program, EPMR, which performs automated six-dimensional MR searches using an evolutionary optimization algorithm. We have examined the limits of effectiveness of this method with regard to search model quality, data quality, and alternative scoring criteria, and we are now exploring a variety of methods for extending this approach to make use of large structural databases. A highly parallel version of EPMR for multi-processor machines and computing clusters has been developed which allows multiple search models to be evaluated simultaneously. The evolutionary search procedure also has been extended to include selection of the optimal member of a set of search models during the course of the evolutionary search. We are now exploring the practicality of searching simultaneously with smaller structural fragments to allow the molecular model to be constructed during the search. The limits of these procedures with respect to database size and search model quality will be discussed.

Index of /ACA/ACA01/abstracts/text

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	W0303.html	12-Apr-2001 11:54	2k
	W0304.html	12-Apr-2001 11:54	3k
	W0305.html	12-Apr-2001 11:54	4k
	W0306.html	12-Apr-2001 11:54	3k
	W0307.html	12-Apr-2001 11:54	3k
	W0308.html	12-Apr-2001 11:54	3k
	W0309.html	12-Apr-2001 11:54	2k
	W0310.html	12-Apr-2001 11:54	2k
	W0311.html	12-Apr-2001 11:54	3k
	W0312.html	12-Apr-2001 11:54	4k
	W0313.html	12-Apr-2001 11:54	2k
	W0314.html	12-Apr-2001 11:54	2k
	W0315.html	12-Apr-2001 11:54	2k
	W0316.html	12-Apr-2001 11:54	2k
	W0317.html	12-Apr-2001 11:54	4k
	W0318.html	18-Apr-2001 14:15	3k
	W0319.html	12-Apr-2001 11:54	3k
	W0320.html	12-Apr-2001 11:54	4k
	W0321.html	12-Apr-2001 11:54	2k
	W0322.html	12-Apr-2001 11:54	3k
	W0323.html	12-Apr-2001 11:54	3k
	W0324.html	12-Apr-2001 11:54	3k
	W0325.html	12-Apr-2001 11:54	3k
	W0326.html	12-Apr-2001 11:54	3k
	W0327.html	12-Apr-2001 11:54	3k
	W0328.html	12-Apr-2001 11:54	3k
	W0329.html	12-Apr-2001 11:54	4k

 W0330.html	12-Apr-2001 11:54	4k
 W0331.html	12-Apr-2001 11:54	4k
 W0332.html	12-Apr-2001 11:54	3k
 W033200.gif	12-Apr-2001 07:55	3k
 W0333.html	12-Apr-2001 11:54	3k
 W033300.gif	12-Apr-2001 07:55	2k
 W033301.gif	12-Apr-2001 07:55	2k
 W033302.gif	12-Apr-2001 07:55	1k
 W0334.html	12-Apr-2001 11:54	3k
 W033400.gif	12-Apr-2001 07:55	16k
 W0335.html	12-Apr-2001 11:54	3k
 W033500.gif	12-Apr-2001 07:55	1k
 W033501.gif	12-Apr-2001 07:55	11k
 W0336.html	12-Apr-2001 11:54	2k
 W0337.html	12-Apr-2001 11:54	3k
 W033700.gif	12-Apr-2001 11:40	1k
 W033701.gif	12-Apr-2001 11:40	1k
 W0338.html	12-Apr-2001 11:54	3k
 W0339.html	12-Apr-2001 11:54	3k
 W0340.html	12-Apr-2001 11:54	3k
 W0341.html	23-Apr-2001 11:43	4k
 W0342.html	23-Apr-2001 11:43	3k
 W0343.html	23-Apr-2001 11:43	3k
 W0344.html	23-Apr-2001 11:43	1k
 W0345.html	23-Apr-2001 11:43	3k
 W0346.html	12-Apr-2001 17:28	4k
 W0347.html	23-Apr-2001 11:43	2k
 W0348.html	23-Apr-2001 11:43	3k
 W0349.html	23-Apr-2001 11:43	3k
 W0350.html	23-Apr-2001 11:43	3k
 W0351.html	23-Apr-2001 11:43	3k
 W0352.html	12-Apr-2001 11:54	2k
 W0353.html	12-Apr-2001 11:54	3k
 W0354.html	12-Apr-2001 11:54	3k
 W0355.html	12-Apr-2001 11:54	3k

	W0356.html	12-Apr-2001 11:54	3k
	W0357.html	12-Apr-2001 11:54	2k
	W0358.html	23-Apr-2001 11:43	3k
	W035800.gif	23-Apr-2001 09:39	1k
	W035801.gif	12-Apr-2001 15:24	1k
	W0359.html	12-Apr-2001 11:54	2k
	W0360.html	12-Apr-2001 11:54	2k
	W0361.html	12-Apr-2001 11:54	2k
	W0362.html	12-Apr-2001 11:54	3k
	W0363.html	12-Apr-2001 11:54	3k
	W0364.html	12-Apr-2001 11:54	3k
	W0365.html	23-Apr-2001 11:43	4k
	W0366.html	12-Apr-2001 11:54	3k
	W0367.html	23-Apr-2001 11:43	3k
	W0368.html	23-Apr-2001 11:43	3k
	W0369.html	12-Apr-2001 11:54	3k
	W0370.html	23-Apr-2001 11:43	3k
	W0371.html	23-Apr-2001 11:43	3k
	W0372.html	23-Apr-2001 11:43	3k
	W0373.html	23-Apr-2001 11:43	3k
	W0374.html	18-Apr-2001 14:15	2k
	W0375.html	23-Apr-2001 11:43	3k
	W0376.html	26-Apr-2001 13:28	3k
	W0377.html	23-Apr-2001 11:43	3k
	W0378.html	26-Apr-2001 13:28	3k
	W0379.html	26-Apr-2001 13:28	3k
	W0380.html	12-Apr-2001 11:54	3k
	W0381.html	12-Apr-2001 11:54	4k
	W0382.html	12-Apr-2001 11:54	3k
	W0383.html	12-Apr-2001 11:54	2k
	W0384.html	12-Apr-2001 11:54	2k
	W0385.html	18-Apr-2001 14:15	3k
	W0386.html	23-Apr-2001 11:43	2k
	W0387.html	23-Apr-2001 11:43	3k
	W0388.html	18-Apr-2001 14:15	2k

	W0389.html	18-Apr-2001 14:15	3k
	W0390.html	18-Apr-2001 14:15	3k
	W0391.html	18-Apr-2001 14:15	4k
	W0392.html	18-Apr-2001 14:15	3k
	W0393.html	26-Apr-2001 13:28	4k
	W0394.html	26-Apr-2001 13:28	3k
	W039400.gif	25-Apr-2001 08:04	6k
	W039401.gif	25-Apr-2001 08:04	127k
	W039402.gif	25-Apr-2001 08:04	127k
	W0395.html	14-May-2001 15:07	3k
	W0396.html	27-Apr-2001 13:39	3k
	W0397.html	14-May-2001 15:07	2k
	W0398.html	14-May-2001 15:07	3k
	W0399.html	14-May-2001 15:07	3k
	W0400.html	14-May-2001 15:07	2k
	W0401.html	14-May-2001 15:07	2k
	W0404.html	25-Jun-2001 15:48	4k
	W0405.html	25-Jun-2001 15:48	3k
	W0406.html	25-Jun-2001 15:48	4k
	W0407.html	27-Jun-2001 10:54	3k
	W0408.html	27-Jun-2001 10:54	2k
	W0409.html	27-Jun-2001 10:54	4k
	W0410.html	27-Jun-2001 10:54	2k
	W0411.html	27-Jun-2001 10:54	2k
	W0412.html	27-Jun-2001 10:54	2k
	W0413.html	27-Jun-2001 10:54	3k
	W0414.html	27-Jun-2001 10:54	2k
	W0415.html	27-Jun-2001 10:54	4k
	W0416.html	25-Jun-2001 15:48	3k
	W0417.html	25-Jun-2001 15:48	3k
	W0418.html	25-Jun-2001 15:48	3k
	W0419.html	25-Jun-2001 15:48	2k
	W0420.html	25-Jun-2001 15:48	4k